# Neutron shell structure and deformation in neutron-drip-line nuclei

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## Abstract

Neutron shell-structure and the resulting possible deformation in the neighborhood of neutrondrip-line nuclei are systematically discussed, based on both bound and resonant neutron oneparticle energies obtained from spherical and deformed Woods-Saxon potentials. Due to the unique behavior of weakly-bound and resonant neutron one-particle levels with smaller orbital angularmomenta  $\ell$ , a systematic change of the shell structure and thereby the change of neutron magicnumbers are pointed out, compared with those of stable nuclei expected from the conventional i-j shell-model. For spherical shape with the operator of the spin-orbit potential conventionally used, the  $\ell_i$  levels belonging to a given oscillator major shell with parallel spin- and orbital-angularmomenta tend to gather together in the energetically lower half of the major shell, while those levels with anti-parallel spin- and orbital-angular-momenta gather in the upper half. The tendency leads to a unique shell structure and possible deformation when neutrons start to occupy the orbits in the lower half of the major shell. Among others, the neutron magic-number N=28 disappears and N=50 may disappear, while the magic number N=82 may presumably survive due to the large  $\ell = 5$  spin-orbit splitting for the  $1h_{11/2}$  orbit. On the other hand, an appreciable amount of energy gap may appear at N=16 and 40 for spherical shape, while neutron-drip-line nuclei in the region of neutron number above N=20, 40 and 82, namely N  $\approx$  21-28, N  $\approx$  41-54, and N  $\approx$  83-90, may be quadrupole-deformed though the possible deformation depends also on the proton number of respective nuclei.

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#### I. INTRODUCTION

Thanks to the development of various facilities of radioactive nuclear ion beam, the knowledge of nuclei far away from the stability line has recently been much increased. Though the neutron drip line has so far been experimentally pinned down up till the oxygen (Z=8) isotope, at the moment the experimental knowledge of nuclei with Z>8 close to the neutron drip line is quickly increasing.

The study of unstable nuclei, especially neutron-drip-line nuclei which contain very weakly bound neutrons, has opened a new field in the study of the structure of finite quantum-mechanical systems. The study is important not only for the interests in nuclear astrophysics namely for the understanding of the production of energy and the synthesis of elements in stars and during stellar events, but also for giving the opportunity for learning the properties of the Fermion system with very loosely-bound particles, some density of which can extend to the region far outside the region of the main density of the system. Various exciting study of man-made finite quantum-mechanical systems, such as clusters of atoms and quantum dots, has recently been made possible, however, those systems are so far limited to be well bound so that the related potentials are in a good approximation simulated by a harmonic-oscillator. Since the nucleon separation energy in stable nuclei is 7-10 MeV, the spectroscopic analysis around the ground state of stable nuclei has been successfully carried out also in terms of harmonic-oscillator wave-functions. Correspondingly, most of systematic nuclear shell-model calculations are so far carried out using harmonic-oscillator wave-functions.

The study of one-particle motion in deformed potentials is the basis for understanding the structure of deformed nuclei. Since the Fermi level of drip line nuclei lies close to the continuum, both weakly-bound and positive-energy one-particle levels play a crucial role in the many-body correlations of those nuclei. Among an infinite number of one-particle levels at a given positive energy, only some selected levels related to one-particle resonant levels will be important for the understanding of the properties of bound states of drip-line nuclei.

The behavior of s neutrons is an extreme example because the barrier coming from either centrifugal or Coulomb potentials is absent. Therefore, for example, as the separation energy approaches zero, the probability of s neutrons staying inside the nuclei approaches zero. When a larger part of a bound one-particle wave-function lies outside the nuclear potential, the one-particle eigen energy becomes less sensitive to the potential provided by

the well-bound nucleons in the system. In contrast, the wave functions of weakly-bound but large- $\ell$  neutrons stay mostly inside the nuclear potential, due to the high barrier coming from the centrifugal potential, of which the height is proportional to  $\ell(\ell+1)$ . Consequently, when the potential changes (or the neutron number for a given proton number approaches the neutron-drip-line) so that one-particle energies of last bound neutrons approach zero, the binding energy of larger- $\ell$  neutrons, which is more sensitive to the strength of the potential, decreases much faster than that of smaller- $\ell$  neutrons. The height of the centrifugal potential also affects sharply the properties of one-particle resonant levels. Thus, the same behavior of  $\ell$ -dependence as that of weakly-bound neutron energies is obtained also for lower-lying neutron one-particle resonant energies, as shown in Ref. [1–3]. This  $\ell$ -dependent behavior of one-particle energies on the potential strength leads to a systematic change of the shell structure in both weakly-bound and resonant neutron one-particle energies compared with the shell structure of strongly-bound neutrons [4].

Using the numerical result of the self-consistent mean-field calculations with effective interactions used in stable nuclei while limiting the spherical system in a large box, one-particle spectra of bound nucleons in spherical drip-line-nuclei were studied in Ref. [5]. And, some systematic change of shell structure in bound neutron energies of spherical neutron drip-line nuclei was obtained, which is similar to that of the present work found at  $\beta = 0$  except the conclusion in Ref. [5] that the presence of magic gaps at the neutron number N = 28, 50 and 82 does not appreciably change as one approaches the neutron-drip-line.

Taking the (N=2) sd- and (N=3) pf-shells where N expresses the harmonic-oscillator principle quantum-number, the systematic change of shell structure due to the unique behavior of one-particle energies of weakly-bound or resonant levels with small  $\ell$  is briefly explained in the following. In stable sd-shell nuclei, it is well-known that the relation of one-particle energies is such that  $\epsilon(1d_{5/2}) < \epsilon(2s_{1/2}) < \epsilon(1d_{3/2})$ , which agrees with experimental information. However, in lighter neutron-rich nuclei, in which the  $2s_{1/2}$  level becomes very weakly bound, the relation  $\epsilon(2s_{1/2}) \approx \epsilon(1d_{5/2}) < \epsilon(1d_{3/2})$  is expected, which leads to the new magic number N=16 [6]. In fact, the appearance of the N = 16 neutron magic number for unstable nuclei together with a weakening of the shell closure at N = 20 and 28 was mentioned already in 1975 [7] based on the self-consistent calculations using the energy density formalism with pairing interaction. On the other hand, in heavier nuclei where neutrons in the sd-shell are strongly bound, the relation  $\epsilon(1d_{5/2}) < \epsilon(1d_{3/2}) < \epsilon(2s_{1/2})$  is obtained from

both Hartree-Fock calculations and eigenvalues of Woods-Saxon potentials with a practical strength of spin-orbit potential. Similarly, if we take an example of the pf-shell, the relation  $\epsilon(1f_{7/2}) < \epsilon(1f_{5/2}) < \epsilon(2p_{3/2}) < \epsilon(2p_{1/2})$  is obtained in the case of strongly-bound pf-neutrons. For stable pf-shell nuclei, the relation  $\epsilon(1f_{7/2}) < \epsilon(2p_{3/2}) < \epsilon(1f_{5/2}) \approx \epsilon(2p_{1/2})$  is known. However, when one-particle levels of  $1f_{7/2}$  and  $2p_{3/2}$  become very weakly-bound or resonant, the relation  $\epsilon(1f_{7/2}) \approx \epsilon(2p_{3/2})$  appears. The relation leads to the disappearance of the magic number N=28 [4] and, moreover, nuclei with some neutrons in the almost degenerate  $f_{7/2}$  and  $p_{3/2}$  shells, which couple strongly each other by quadrupole-quadrupole interaction, may be easily quadrupole deformed. The degeneracy can well be responsible for the presence of "island of inversion". It has been known that the presence of only like nucleons in a large single-j-shell can hardly lead to quadrupole deformation. On the other hand, the presence of like nucleons in several nearly degenerate j-shells, which couple strongly each other by quadrupole-quadrupole interaction, may lead to quadrupole deformation.

In axially-symmetric quadrupole-deformed nuclei the role of smaller- $\ell$  neutrons for spherical shape is replaced by neutrons with smaller  $\Omega$  values, where  $\Omega$  denotes the angular momentum component of neutrons along the axially-symmetry axis. For example, the smallest possible angular-momentum component of  $\Omega^{\pi} = 1/2^{+}$  orbits is  $s_{1/2}$ , which becomes always the overwhelming component of angular-momentum in neutron one-particle wave-functions with  $\Omega^{\pi} = 1/2^{+}$  as the binding energy of the neutron approaches zero [1, 8]. In the case that the smallest orbital angular-momentum is not equal to zero, it depends on the properties of respective orbits how the component of the smallest orbital angular-momentum becomes dominant in one-particle wave-functions when the binding energy approaches zero [1]. Since all spherical one-particle orbits with positive parity  $(s_{1/2}, d_{3/2}, d_{5/2}, ...)$  have an  $\Omega^{\pi} = 1/2^+$ component, the shell structure change for deformed shape close to the continuum due to the unique property of  $s_{1/2}$  orbit is expected to occur more often compared with the case of spherical shape. It is the most convenient way to see the shell structure of deformed nuclei to plot one-particle energies as a function of quadrupole deformation (Nilsson diagram) [9]. Therefore, in this article Nilsson diagrams that are relevant to some possible neutron-dripline nuclei related to neutron magic numbers in stable nuclei are presented. The change of nuclear shell structure for neutrons is seen in both bound and resonant one-particle energies in Nilsson diagrams.

In Sec. II main points of our model are briefly summarized, while numerical results are

presented in Sec. III. Conclusions and discussions are given in Sec. IV.

### II. MODEL

In order to solve the eigenvalue [1] and eigenphase [2, 3] problems for neutron one-particle bound and resonant levels, respectively, as a function of axially-symmetric quadrupole deformation, the coupled differential equations obtained from the Schrödinger equation are integrated in coordinate space with correct asymptotic behavior at  $r=R_{max}$ , where  $R_{max}$  is so large that both the nuclear potential and the coupling term are negligible. In this way one-particle resonant energy in deformed nuclei can also be estimated without any ambiguity. For  $\beta \neq 0$  the resonant energy is defined as the energy, at which one of the eigenphases increases through  $\pi/2$  as the energy increases [2, 3, 10]. One-particle resonance is absent if none of eigenphases increase through  $\pi/2$  as the energy increases. For example, neutron one-particle resonant state with  $\Omega^{\pi}=1/2^+$  is not obtained as far as the major component of the one-particle wave-function comes from  $\ell=0$ , because an  $\Omega^{\pi}=1/2^+$  level with an appreciable amount of the  $\ell=0$  component can very quickly decay via the  $\ell=0$  channel. Since the height of the centrifugal barrier decreases for a larger nuclear radius, the unique behavior of  $\ell=1$  components contained in the  $\Omega^{\pi}=1/2^-$  and  $3/2^-$  orbits will be more easily seen in heavier nuclei.

On the other hand, since the height of the centrifugal barrier is proportional to  $\ell(\ell+1)$ , at a given positive energy for a given potential the width of a one-particle resonant level is larger for the level with smaller orbital angular-momentum. As the energy increases the width of a given resonant level becomes larger, and finally at a certain energy the one-particle level with a given  $\ell$  is no longer obtained as a resonant level. For simplicity, the calculated widths of one-particle resonant levels are not given in the present article, since the widths are not a major subject in this work.

Though weakly-bound neutrons in nuclei close to the neutron drip line have a contribution especially to the tail of the self-consistent nuclear potentials, the major part of the nuclear potential is provided by well-bound nucleons, especially by strongly-bound protons in the case of neutron-rich nuclei. Therefore, for simplicity, in this article the parameters of Woods-Saxon potentials are taken from the standard ones (see p.239 of [11]). Namely, the diffuseness a=0.67 fm, the radius  $r_0A^{1/3}$  where  $r_0=1.27$  fm, the depth of the Woods-Saxon potential for

neutrons is

$$V = -51 + 33 \frac{N - Z}{A} \qquad \text{MeV} \tag{1}$$

and the spin-orbit potential is expressed by

$$V_{\ell s} = -0.44V \left(\vec{\ell} \cdot \vec{s}\right) r_0^2 \frac{1}{r} \frac{d}{dr} f(r) \qquad \text{MeV}$$
 (2)

where

$$f(r) = \frac{1}{1 + exp(\frac{r-R}{a})}\tag{3}$$

It is noted that the neutron potential for nuclei with a neutron excess is shallower than that for N=Z nuclei. In fact, the nuclear potential with the above set of parameters is found to approximately reproduce the position of the neutron drip line, which is expected from presently available experimental data.

In the discussion of possible deformation of given nuclei examining the Nilsson diagram we use the following empirical facts: (a) If pair correlation plays a minor role, the presence of neutrons in almost degenerate  $\ell_j$  shells around the Fermi level may make the system deformed since those neutrons have a possibility of gaining energy by breaking spherical symmetry (Jahn-Teller effect); (b) In order to obtain a deviation from spherical shape, the energies of one-particle levels just below and on the Fermi level in the Nilsson diagram need to be mostly decreasing (downward-going) for  $\beta = 0 \rightarrow \beta \neq 0$  so that the system gains the energy by deformation [9]; (c) The presence of only like nucleons in a large single-j-shell may not be sufficient to deform the system, though the presence of both neutrons and protons in a given single-j-shell may induce some quadrupole deformation. Examples are: no observed deformed nuclei both in the  $_{38}$ Sr and  $_{40}$ Zr isotopes due to the occupation of the  $_{199/2}$  shell by neutrons [12], and in the  $_{18}Ar$  and  $_{20}$ Ca isotopes due to the occupation of the  $_{1}f_{7/2}$  shell by neutrons; (d) Only prolate deformation is discussed, since it is empirically known that prolate deformation is overwhelmingly dominant among deformed nuclei though the absolute dominance is not yet fully understood [13].

## III. NUMERICAL RESULTS

Though the near degeneracy of both the  $1d_{5/2} - 2s_{1/2}$  levels in the N=2 oscillator shell and that of  $1f_{7/2} - 2p_{3/2}$  levels in the N=3 shell of the spherical potential in neutron-drip-line nuclei as well as the resulting possible deformation are partly discussed in Ref. [4], in the

following we include a brief description of those cases for completeness. The two remaining  $n\ell_j$  levels,  $1f_{5/2}$  and  $2p_{1/2}$ , in the N=3 oscillator major shell other than the  $1f_{7/2}$  and  $2p_{3/2}$ levels, in which spin and orbital angular momenta are anti-parallel, may become also almost degenerate around the Fermi level of certain nuclei. Nevertheless, the degeneracy may not lead to a deformation, because those levels lie in the second half of the N=3 major shell and, then, the general behavior of the deformed one-particle energies originating from those levels in the spherical limit is energetically upward-going for  $\beta = 0 \rightarrow \beta \neq 0$ . The relation between deformation of the system and upward-going (or downward-going) energy levels in the Nilsson diagram is known already in the study of stable rare-earth nuclei [9]. Namely, energetically downward-going one-particle levels for  $\beta = 0 \rightarrow \beta > 0$  (prolate shape) around  $N \gtrsim 88-90$  that lead to stable deformed rare-earth nuclei, end at  $N \approx 110$ , around which the observed deformation of stable rare-earth nuclei also ends. (See, for example, Fig.5-3 of [9].) As is seen in the following, the shell structure unique in neutron weakly-bound and resonant levels leads to the bunching of one-particle levels in a given N major shell for spherical shape: levels with parallel spin- and orbital-angular-momenta gather together in the lower half of the major shell, while levels with anti-parallel spin- and orbital-angular-momenta gather in the upper half shell. Levels within the respective groups couple each other strongly by spinindependent quadrupole-quadrupole interaction. However, we note that there is a difference between the two groups concerning the possible deformation. Namely, having neutrons in the nearly degenerate levels with parallel spin- and orbital- angular-momenta may make the system deformed, because one-particle energies in the lower half of a given N major shell are in general decreasing for  $\beta = 0 \rightarrow \beta \neq 0$ , as can be seen from the Nilsson diagram. Since the levels belonging to each group have different orbital angular-momenta, the occurrence of near degeneracy depends on the actual strength of spin-orbit splitting and the values of relevant orbital angular momenta. As seen in the  $1h_{11/2}$  orbit of Fig. 4, the highest-j level with parallel spin- and orbital-angular-momenta tends to go out of the group of degenerate levels in heavier nuclei.

# A. Near degeneracy of $1d_{5/2}$ and $2s_{1/2}$ levels

In Fig. 1 we show the Nilsson diagram for neutrons, in which parameters of the Woods-Saxon potential are chosen for the nucleus  ${}^{18}_{6}$ C<sub>12</sub>. It is noted that the observed ground-

state spins of nuclei  ${}_{6}^{15}$ C<sub>9</sub>,  ${}_{6}^{17}$ C<sub>11</sub>, and  ${}_{6}^{19}$ C<sub>13</sub> are  $1/2^+$ ,  $3/2^+$ , and  $1/2^+$ , respectively, and are most easily understood in terms of prolate deformation for  $\beta > 0.1$ , where the last odd neutron occupies the  $\Omega^{\pi} = 1/2^+$ ,  $3/2^+$  and  $1/2^+$  levels that correspond to the 9th, 11th, and 13th neutron one-particle levels, respectively, assuming that the respective even-even core nucleons occupy pair-wise the lower-lying Nilsson one-particle levels and couple to  $I^{\pi} = K^{\pi} = 0^+$ . For some experimental evidence for the deformation of those C-isotopes, see Refs. [14, 15]. At  $\beta = 0$  the calculated energy difference between the  $2s_{1/2}$  and  $1d_{5/2}$  levels in Fig. 1 is only 509 keV. In contrast, a large energy gap for spherical shape ( $\beta = 0$ ) appears at N = 16, since the calculated  $1d_{3/2}$  resonant energy is 4.36 MeV.

## B. Near degeneracy of $1f_{7/2}$ and $2p_{3/2}$ levels

In Fig. 2 the Nilsson diagram for neutrons is shown, in which parameters of the Woods-Saxon potential are chosen for the nucleus  $^{34}_{12}\mathrm{Mg}_{22}$ . At  $\beta=0$  the calculated energy difference between the very weakly bound  $1f_{7/2}$  level and very low-lying one-particle resonant  $2p_{3/2}$ level is only 387 keV, which clearly indicates that the N = 28 energy gap at  $\beta$ =0 disappears in neutron-drip-line nuclei. This near degeneracy of the two levels, which couple strongly each other by spin-independent quadrupole-quadrupole interaction, may lead to the deformation of the system with N  $\approx$  21-28, as a result of the Jahn-Teller effect. In particular, odd-A nuclei with N=21 such as  $^{33}_{12}Mg_{21}$  [16, 17] and  $^{31}_{10}Ne_{21}$  [18] are observed to be deformed, being consistent with the strongly down-sloping Nilsson one-particle levels with  $\Omega^{\pi}=1/2^{-}$  and  $3/2^-$  for  $\beta > 0$ , which originate from the  $1f_{7/2}$  shell in the spherical limit ( $\beta = 0$ ). Neutrondrip-line nuclei with N = 21-28 can well be deformed though the possible deformation depends also on the proton number of respective nuclei. Examining the Nilsson diagram for protons it is seen that the proton numbers Z = 9 (F), 10 (Ne), 11(Na) and 12 (Mg) may prefer some deformation since the energies of the two lowest-lying Nilsson one-proton levels in the sd-shell decrease sharply as  $\beta=0$   $\rightarrow$   $\beta\neq0$ . The recent experimental information on the Mg isotope with N = 21-26 [19] seems to go well with this interpretation using the Nilsson diagram. Indeed, this near degeneracy of the  $1f_{7/2}$  and  $2p_{3/2}$  levels can be an important element for creating "island of inversion". In other words, heavier nuclei in the "island of inversion" could survive inside the neutron-drip-line thanks to the deformation.

From Fig.2 it is also seen that at  $\beta=0$  the well-bound  $2s_{1/2}$  level lies approximately in the

middle of the  $2d_{5/2}$  and  $2d_{3/2}$  levels, in contrast to the sd-shell level scheme shown in Fig.1.

## C. Near degeneracy of $1g_{9/2}$ , $3s_{1/2}$ and $2d_{5/2}$ levels

In Fig. 3 the Nilsson diagram for neutrons is shown, in which parameters of the Woods-Saxon potential are chosen for the nucleus  $^{66}_{22}\mathrm{Ti}_{44}$ . A considerable amount of energy gap appears at N = 40 for spherical shape, while the possible location of the  $3s_{1/2}$  level slightly above zero (indicated by the open circle in Fig. 3) is obtained from the extrapolation of the bound one-particle energy level with  $\Omega^{\pi}=1/2^+$  for  $\beta>0.12$  denoted by the solid curve in Fig. 3, which reaches zero at  $\beta=0.12$ , since the continuation of the one-particle resonant level to the region of  $\beta<0.12$  cannot be obtained due to the predominant  $\ell=0$  component of the orbit. Thus, the calculated  $1g_{9/2}$ ,  $3s_{1/2}$  and  $2d_{5/2}$  levels, which are the three  $n\ell_j$  levels belonging to the N=4 oscillator shell with parallel spin- and orbital-angular-momenta and couple strongly each other by spin-independent quadrupole-quadrupole interaction, lie within 1.43 MeV. This means that the energy gap at the magic number N = 50 clearly disappears.

The strong quadrupole coupling of these three levels can be seen from the Nilsson diagram in Fig. 3. For example, the lowest-lying one-particle level with  $\Omega^{\pi}=1/2^{+}$  for  $\beta>0$ , which is connected to the  $1g_{9/2}$  shell at  $\beta=0$ , contains a considerable amount of  $3s_{1/2}$  and  $2d_{5/2}$  components already at moderate values of  $\beta$ . This can be seen from the comparison between the slopes of the  $\Omega^{\pi}=1/2^{+}$  curve for  $\beta>0$  and the  $\Omega^{\pi}=9/2^{+}$  curve for  $\beta<0$ , both of which originate from the  $1g_{9/2}$  level at  $\beta=0$ . The wave-function of the  $\Omega^{\pi}=9/2^{+}$  orbit is almost pure  $1g_{9/2}$  in the present range of  $\beta$ -values since there is no  $\Omega^{\pi}=9/2^{+}$  one-particle orbit in the neighborhood. If both orbits,  $\Omega^{\pi}=1/2^{+}$  for  $\beta>0$  and  $\Omega^{\pi}=9/2^{+}$  for  $\beta<0$ , consist only of a single-j-shell, namely  $g_{9/2}$ , then, the absolute magnitude of the slope,  $|\frac{d\epsilon_{\Omega}}{d\beta}|$ , of the  $\Omega^{\pi}=9/2^{+}$  level is a factor 2 larger than that of the  $\Omega^{\pi}=1/2^{+}$  level. On the other hand, for a pure harmonic oscillator potential (namely the strong mixing limit) the former is a half (= 0.5) of the latter. In Fig. 3 the ratio of the former to the latter is about 2, of course, for  $|\beta| << 1$ , while the absolute magnitude of the slope of the  $\Omega^{\pi}=1/2^{+}$  energy level becomes larger than that of the  $\Omega^{\pi}=9/2^{+}$  energy level already at  $|\beta|$  smaller than 0.3.

The near degeneracy of these three levels,  $1g_{9/2}$ ,  $3s_{1/2}$  and  $2d_{5/2}$ , corresponds to that of the  $1f_{7/2}$  and  $2p_{3/2}$  levels discussed in the previous subsection, which leads to "the island"

of inversion". First of all, neutron-drip-line nuclei with N = 41 is likely to be deformed, though the possible deformation depends also on the proton number of respective nuclei. The ground-state spin of neutron-drip-line nuclei with N = 41 can be either  $1/2^+$  or  $5/2^+$  or  $1/2^-$  or  $3/2^-$  depending on  $\beta$ -values if they are prolately deformed, instead of  $9/2^+$  expected for spherical shape. Secondly, a system having several neutrons in these  $(1g_{9/2} - 3s_{1/2} - 2d_{5/2})$  almost degenerate shells such as N  $\approx 41 - 54$  is likely to be deformed in a similar way to "the island of inversion", when pairing interaction plays a minor role. See the fourth paragraph of Sec. IV for the discussion of the role of pairing interaction in the determination of the shape of neutron-drip-line nuclei.

The near degeneracy of the  $1g_{9/2}$  level with other two levels has occurred for the phenomenological strength of the spin-orbit splitting which is not yet so strong for the  $1g_{9/2}$  orbit. As is seen in the next subsection, in the N=5 oscillator major shell the spin-orbit splitting of the  $1h_{11/2}$  level is so strong that the similar degeneracy of all levels with parallel spin- and orbital-angular-momenta belonging to the N=5 major shell can hardly occur.

The remaining two levels in the N=4 oscillator major shell,  $1g_{7/2}$  and  $2d_{3/2}$ , may be almost degenerate around the Fermi level of certain neutron-drip-line nuclei. However, it may be difficult to gain energies by deforming those nuclei which have neutrons in those two levels, since one-particle energies originating from the  $1g_{7/2}$  and  $2d_{3/2}$  levels are located in the second half of the N=4 major shell and thus the energies of the majority of one-particle levels increase for  $\beta=0 \rightarrow \beta \neq 0$ .

# D. Near degeneracy of $1h_{11/2}$ , $2f_{7/2}$ and $3p_{3/2}$ levels ?

In Fig. 4 the Nilsson diagram for neutrons is shown, in which parameters of the Woods-Saxon potential are chosen for the nucleus  $^{126}_{44}$ Ru<sub>82</sub>. A considerable amount of the energy gap remains at N = 82 for spherical shape due to the large spin-orbit splitting of the  $\ell$  = 5 level,  $1h_{11/2}$ , while the very weakly-bound  $2f_{7/2}$  and  $3p_{3/2}$  levels are very close-lying. The calculated energy distance between the two levels is only 419 keV.

The set of three levels,  $1h_{11/2}$ ,  $2f_{7/2}$  and  $3p_{3/2}$ , which strongly couple each other by spinindependent quadrupole-quadrupole interaction, is the set of the N=5 oscillator major shell analogous to the set of three levels,  $1g_{9/2}$ ,  $2d_{5/2}$ , and  $3s_{1/2}$ , of the N=4 major shell discussed in the previous subsection. In the latter case a deformation may be energetically preferred for the system where some neutrons occupy the set of levels due to the Jahn-Teller effect, while in the present case a deformation may not be preferred since the one-particle levels for a moderate size of prolate shape in Fig. 4 originating from  $1h_{11/2}$  seem to mostly maintain the feature of the single-j-shell. On the other hand, the occupation of the almost degenerate shells,  $2f_{7/2}$  and  $3p_{3/2}$ , by some neutrons may lead to a deformed system for N = 83-90 when the proton part of respective nuclei is energetically easily deformable and the pairing interaction plays a minor role. For example, the nucleus  $^{127}_{44}$ Ru<sub>83</sub> may be deformed, in a similar way to the nucleus  $^{33}_{12}$ Mg<sub>21</sub> in the "island of inversion" (see Fig. 2.). If it is deformed the ground-state spin of the N = 83 nucleus is likely to be  $1/2^-$  or  $3/2^-$  or  $3/2^+$  depending on  $\beta$ -values instead of  $7/2^-$  expected for spherical shape.

In contrast to the three levels with parallel spin- and orbital-angular-momenta belonging to the N=5 oscillator major shell, filling the three levels,  $1h_{9/2}$ ,  $2f_{5/2}$  and  $3p_{1/2}$ , by some neutrons which belong to the same major shell with anti-parallel spin- and orbital-angular-momenta may not lead to deformation, in spite of the fact that those three levels may become almost degenerate around the Fermi level of certain nuclei as can be guessed from Fig. 4.

#### IV. CONCLUSIONS AND DISCUSSIONS

A systematic study of the shell structure and the resulting possible deformation around neutron-drip-line nuclei has been carried out based on both bound and resonant neutron one-particle energies obtained from phenomenological Woods-Saxon potentials. In order to solve the eigenvalue and eigenphase problems for neutron one-particle bound and resonant levels, respectively, for a given deformed potential, the coupled differential equations obtained from the Schrödinger equation are integrated in coordinate space with correct asymptotic behavior. The coupling of a bound (or resonant) one-particle level with other levels, which are not obtained as resonant one-particle levels, is also properly taken into account in the method of the present work.

For spherical shape with the operator of the spin-orbit potential conventionally used, weakly-bound and/or low-lying resonant one-particle levels with parallel spin- and orbital-angular-momenta tend to gather together in the energetically lower half part of the oscillator major shell, while those levels with anti-parallel spin- and orbital-angular-momenta gather

in the upper half. This grouping of energy levels in the spherical potential may lead to a possible deformation when neutrons start to occupy the lower half of the major shell. In contrast, the occupation of the upper half shell by neutrons may not lead to a deformation.

Some concrete result derived from the present study is: the magic numbers N=28 disappears and N=50 may disappear, while the magic number N=82 may presumably survive. For spherical shape an appreciable amount of energy gap appears at N=16 and 40. Neutron-drip-line nuclei in the region of neutron number above N=20, 40 and 82, namely N  $\approx$  21-28 ("island of inversion"), N  $\approx$  41-54, and N  $\approx$  83-90, may be quadrupole-deformed, though the possible deformation depends on the proton number of respective nuclei.

In actual nuclei it is possible that pair correlations may play an important role in the determination of nuclear shape. It is generally understood that the pairing interaction tries to keep nuclei spherical, while the long-range part of two-body interactions such as quadrupole-quadrupole interaction is responsible for deformation. In stable nuclei deformed ground states are usually observed first after several nucleons filled one-particle levels above respective magic numbers. It is qualitatively understood that the presence of the several nucleons makes the deformation induced by the long-range part of the interaction win against the spherical shape preferred by the pairing interaction. However, it is noted that the first two low-lying  $\ell_i$  shells above magic numbers of stable nuclei do not couple strongly each other by the quadrupole-quadrupole interaction because there is a spin-flip between the two  $\ell_j$  shells. For example, the  $2p_{3/2}-1f_{5/2}$  shells just above N = 28, the  $2d_{5/2}-1g_{7/2}$  shells above N = 50 and the  $2f_{7/2}$ -1 $h_{9/2}$  shells above N = 82. Therefore, the deformation-driving effect in stable nuclei by the presence of several nucleons above the magic numbers may be weaker than in the case of neutron-drip-line nuclei. In the latter case the deformationdriving force obtained by filling neutrons in the almost degenerate  $\ell_j$  shells that couple strongly each other by quadrupole-quadrupole interaction may more easily win against the spherical shape preferred by the pairing interaction. On the other hand, the effect of pairing interaction which tries to keep nuclei spherical can be also different in stable and neutrondrip-line nuclei, but the difference does not yet seem to be fully pinned down.

In order to pin down a deformed shape of nuclei, the measurement of both the energy of the lowest  $2^+$  state and  $B(E2; 2_1^+ \to 0^+)$  values in even-even nuclei is important, but to observe the spin-parity of the ground state of odd-A nuclei is often decisive. For example, noting that the proton numbers Z = 21 (Sc), Z = 22 (Ti), Z = 23 (V) and Z = 24 (Cr)

may help to have some deformation as is seen from the fact that the energies of the two lowest-lying Nilsson one-proton levels in the pf-shell decrease strongly as  $\beta = 0 \rightarrow \beta > 0$ , the study of odd-N neutron-drip-line nuclei with N = 41 such as  $^{63}_{22}\mathrm{Ti}_{41}$  is highly desirable. In fact, the spin-parity  $1/2^-$  is already preliminarily assigned to the ground state of  $^{65}_{24}\mathrm{Cr}_{41}$  [20]. On the other hand, the experimental study of neutron-drip-line nuclei with N = 83 may not be possible in a very near future.

The possibility of deformation and the shell structure unique in neutron-drip-line nuclei, which are discussed in this article, should be duly studied by properly carrying out self-consistent Hartree-Fock (HF) calculations with appropriate effective interactions including pairing interaction. However, the effective interactions to be used in HF calculations of neutron-drip-line nuclei are not yet properly fixed. Moreover, such HF calculations have to be done by integrating the coupled differential equations in coordinate space with proper asymptotic behavior of wave functions for  $r = R_{max}$ , at which both nuclear potential and the coupling term are negligible, instead of using the expansion of wave functions in terms of harmonic oscillator bases or confining the system in a finite box. This kind of proper HF calculations are not yet available for neutron-drip-line nuclei. It remains to be seen whether or not neutron-drip-line nuclei with certain neutron numbers are actually deformed as suggested in the present work.

It is noted that the neutron one-particle states obtained from Nilsson diagrams for  $\beta \neq 0$  are those to be recognized as band-head configurations of odd-N nuclei. Thus, rotational states, which are constructed based on those band-head states, should be in principle observed using a proper experimental method, and those high-spin states will have narrow widths if they appear in the low-energy region.

A systematic change of the shell structure in the spherical potential discussed in the present paper is strictly related to the characteristic feature of both the weakly-bound and low-lying resonant one-particle orbits with small  $\ell$  values. The change of the shell structure and the resulting one-particle energies in neutron-drip-line nuclei must be taken into account in the shell-model calculations, when shell model is applied to neutron-drip-line nuclei.

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# Figure captions

- Figure 1: Calculated neutron one-particle energies as a function of quadrupole deformation. Parameters of the Woods-Saxon potential are chosen for the nucleus  ${}^{18}_{6}C_{12}$ . Bound one-particle energies at  $\beta=0$  are -1.17 and -0.66 MeV for the  $1d_{5/2}$  and  $2s_{1/2}$  levels, respectively, while one-particle resonant  $1d_{3/2}$  level is obtained at +4.36 MeV denoted by a filled circle. One-particle resonant levels for  $\beta\neq 0$  are not plotted unless they are important in the present discussion. For simplicity, calculated widths of one-particle resonant levels are not shown. The neutron numbers, 8, 10 and 12, which are obtained by filling all lower-lying levels, are indicated with circles. One-particle levels with  $\Omega=1/2, 3/2$  and 5/2 are expressed by solid, dotted and long-dashed curves, respectively, for both positive and negative parities. The parity of levels can be seen from the  $\ell$ -values denoted at  $\beta=0$ ,  $\pi=(-1)^{\ell}$ .
- Figure 2: Calculated neutron one-particle energies as a function of quadrupole deformation. Parameters of the Woods-Saxon potential are chosen for the nucleus  $^{34}_{12}\text{Mg}_{22}$ . Bound one-particle energies at  $\beta=0$  are  $-9.80,\,-6.84,\,-4.75$  and -0.24 MeV for the  $1d_{5/2},\,2s_{1/2},\,1d_{3/2}$  and  $1f_{7/2}$  levels, respectively, while one-particle resonant  $2p_{3/2}$  and  $1f_{5/2}$  levels are obtained at +0.15 and +6.18 MeV, respectively. The  $2p_{1/2}$  one-particle resonant level is not obtained for the present potential, however, its approximate position at  $\beta=0$  is denoted by an open circle, at which an eigenphase does not reach but comes close to  $\pi/2$ . One-particle resonant levels for  $\beta\neq0$  are not plotted unless they are important in relation to the present interests. The neutron numbers, 20, 22 and 24, which are obtained by filling all lower-lying levels, are indicated with circles. One-particle levels with  $\Omega=1/2,\,3/2,\,5/2$  and 7/2 are expressed by solid, dotted, long-dashed and dot-dashed curves, respectively, for both positive and negative parities.
- Figure 3: Calculated neutron one-particle energies as a function of quadrupole deformation. Parameters of the Woods-Saxon potential are chosen for the nucleus  $^{66}_{22}$ Ti<sub>44</sub>. Bound one-particle energies at  $\beta=0$  are -8.82, -5.54, -3.99, -3.94 and -0.48 MeV for the  $1f_{7/2}, 2p_{3/2}, 2p_{1/2}, 1f_{5/2}$  and  $1g_{9/2}$  levels, respectively, while one-particle resonant  $2d_{5/2}, 1g_{7/2}$  and  $1h_{11/2}$  levels are obtained at +0.96, +5.66 and +7.57 MeV, respectively. The

 $2d_{3/2}$  one-particle resonant level is not obtained for the present potential, however, its approximate position at  $\beta=0$  is denoted by an open circle, at which an eigenphase does not reach but comes close to  $\pi/2$ . The  $3s_{1/2}$  resonant level does not exist in any case, but the open circle at  $\beta=0$  indicates the energy obtained by extrapolating the solid curve of the bound  $\Omega^{\pi}=1/2^{+}$  orbit for  $\beta>0.12$  to  $\beta=0$ , though the calculated solid curve reaches zero at  $\beta=0.12$  and cannot further continue to  $\beta<0.12$ . The major component of the solid curve for  $\epsilon_{\Omega}(<0)\to 0$  is clearly  $3s_{1/2}$ . One-particle resonant levels for  $\beta\neq 0$  are not plotted if they are not relevant for the present discussion. The neutron numbers, 28, 40, 42, 44 and 48, which are obtained by filling all lower-lying levels, are indicated with circles. One-particle levels with  $\Omega=1/2$ , 3/2, 5/2, 7/2 and 9/2 are expressed by solid, dotted, long-dashed, dot-dashed and short-dashed curves, respectively, for both positive and negative parities.

Figure 4: Calculated neutron one-particle energies as a function of quadrupole deformation. Parameters of the Woods-Saxon potential are chosen for the nucleus  $^{126}_{44}$ Ru<sub>82</sub>. Bound one-particle energies at  $\beta=0$  are -7.28, -6.90, -5.70, -5.29, -4.05 -0.48 and -0.06 MeV for the  $2d_{5/2}$ ,  $1g_{7/2}$ ,  $3s_{1/2}$ ,  $2d_{3/2}$ ,  $1h_{11/2}$ ,  $2f_{7/2}$  and  $3p_{3/2}$  levels, respectively, while one-particle resonant  $2f_{5/2}$ ,  $1h_{9/2}$   $1i_{13/2}$  and  $2g_{9/2}$  levels are obtained at +1.71, +1.91, +3.38 and +6.07 MeV, respectively. The  $3p_{1/2}$  one-particle resonant level is not obtained for the present potential, but the open circle at  $\beta=0$  indicates the energy obtained by calculating the spin-orbit splitting of the  $\ell=1$  levels from that of the  $\ell=3$   $(2f_{5/2}$  and  $2f_{7/2}$ ) levels and using the calculated energy of the  $3p_{3/2}$  level. One-particle resonant levels for  $\beta\neq0$  are not plotted if they are not relevant for the present discussion. The neutron numbers 82 and 86, which are obtained by filling all lower-lying levels, are indicated with circles. One-particle levels with  $\Omega=1/2$ , 3/2, 5/2, 7/2, 9/2 and 11/2 are expressed by solid, dotted, long-dashed, dot-dashed, short-dashed and dot-dot-dashed curves, respectively, for both positive and negative parities.







